**Supporting Information**

"Reexamination of Lead(II) Coordination Preferences in Sulfur-Rich Sites: Implications for a Critical Mechanism of Lead Poisoning"

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**Table S1.** Crystal data and structure refinement for $[AsPh_4]_4[Pb(i\text{-mnt})_2]_2$

| | |
|---|---|
| compound | $C_{112}As_4Pb_2N_8S_8H_{80}$ |
| formula weight | 2508.48 |
| crystal system | triclinic |
| space group | $P\bar{1}$ (#2) |
| $a$ (Å) | 11.914(2) |
| $b$ (Å) | 13.355(2) |
| $c$ (Å) | 16.927(3) |
| $V$ (Å$^3$) | 2504.0(7) |
| $Z$ | 1 |
| $d_{calc}$ (g/cm$^{-3}$) | 1.663 |
| cryst. dim. (mm) | 0.64 × 0.13 × 0.06 |
| α | 80.618(3)° |
| $\beta$ | 77.022(3)° |
| $\gamma$ | 73.653(3)° |
| $T$ (K) | 153(1) |
| $\lambda$(Mo Kα) | 0.71069 |
| lin. abs coeff (cm$^{-1}$) | 48.96 |
| transm factors | 0.26572–0.74397 |
| $R(F)^a$ | 0.028 |
| $R_w$ $(F_o^2)^b$ | 0.054 |
| $S$ $(F_o^2)^c$ | 1.53 |

[a] $R(F) = \sum||F_o| - |F_c||/\sum|F_o|$.

[b] $R_w(F_o^2) = [\sum w(F_o^2 - F_c^2)^2/\sum wF_o^4]^{1/2}$

[c] $S = [\sum w(F_o^2 - F_c^2)^2/(N_o\text{-}N_v)]^{1/2}$; $N_o$ = number of observations, $N_v$ = number of variables

**Table S2**. Distances, crystal structure vs. XAS.

| Bond | Distance (Å) (EXAFS) | Distance (Å) (crystallography) | Average Distance (Å) (crystallography) |
|---|---|---|---|
| Pb1-S1 | 2.744 | 2.857 | 2.775 |
| Pb1-S2 | 2.744 | 2.764 | |
| Pb1-S3 | 2.744 | 2.704 | |
| Pb1-S3′ | 3.152 | 3.003 | 3.136 |
| Pb1-S4′ | 3.152 | 3.268 | |
| Pb1-Pb1′ | 3.696 | 3.697 | |

The longest Pb–S distance (3.597 Å in the crystal structure) is not observable in the FT of the EXAFS, as that peak overlaps the strong Pb–Pb interaction (3.696 Å).

**Figure S1.** XANES spectra for all Pb–peptide complexes that were measured.

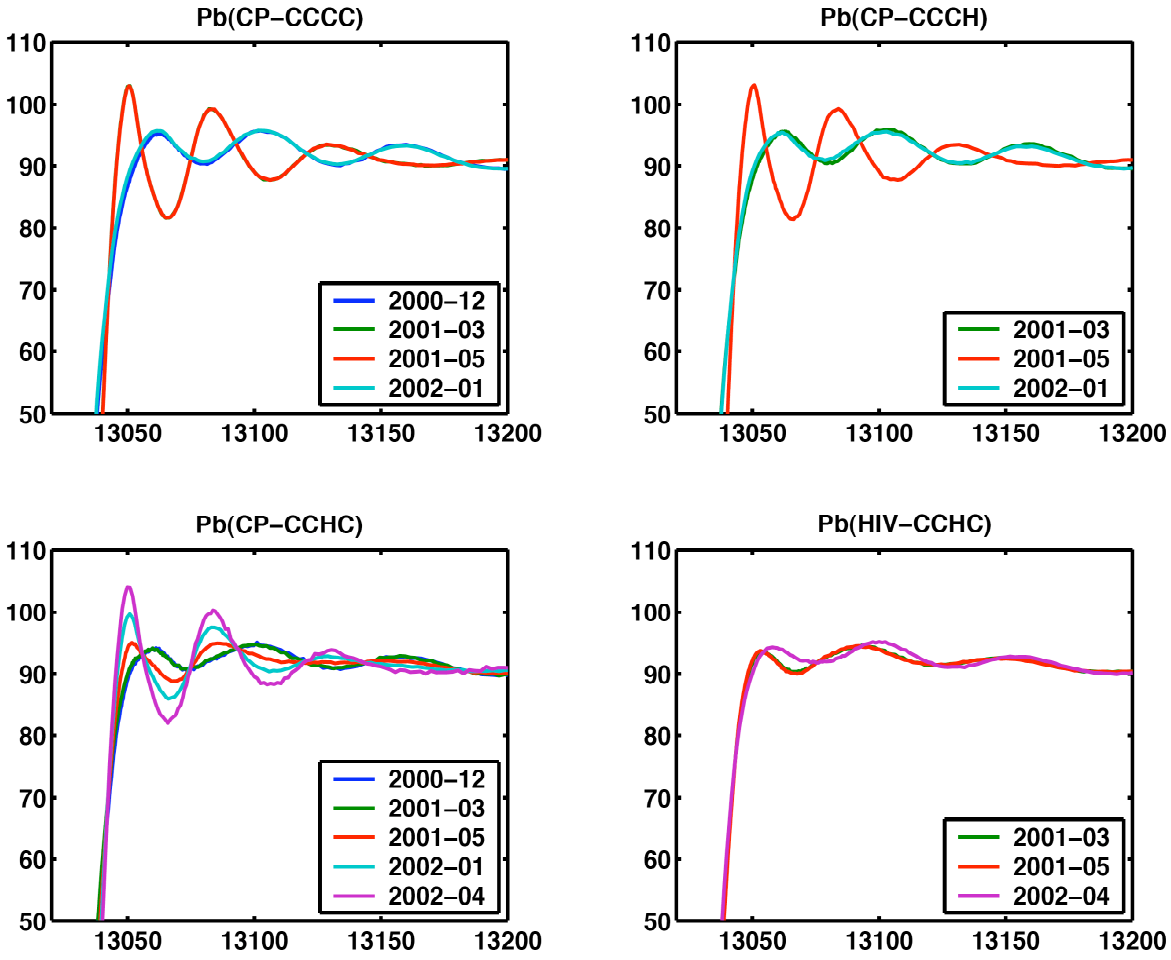

**Figure S2.** FTs of the $k^3$-weighted EXAFS spectra for all the peptides that were measured. For the non-reproducible samples, the FT is consistent with that seen for aqueous Pb(II).

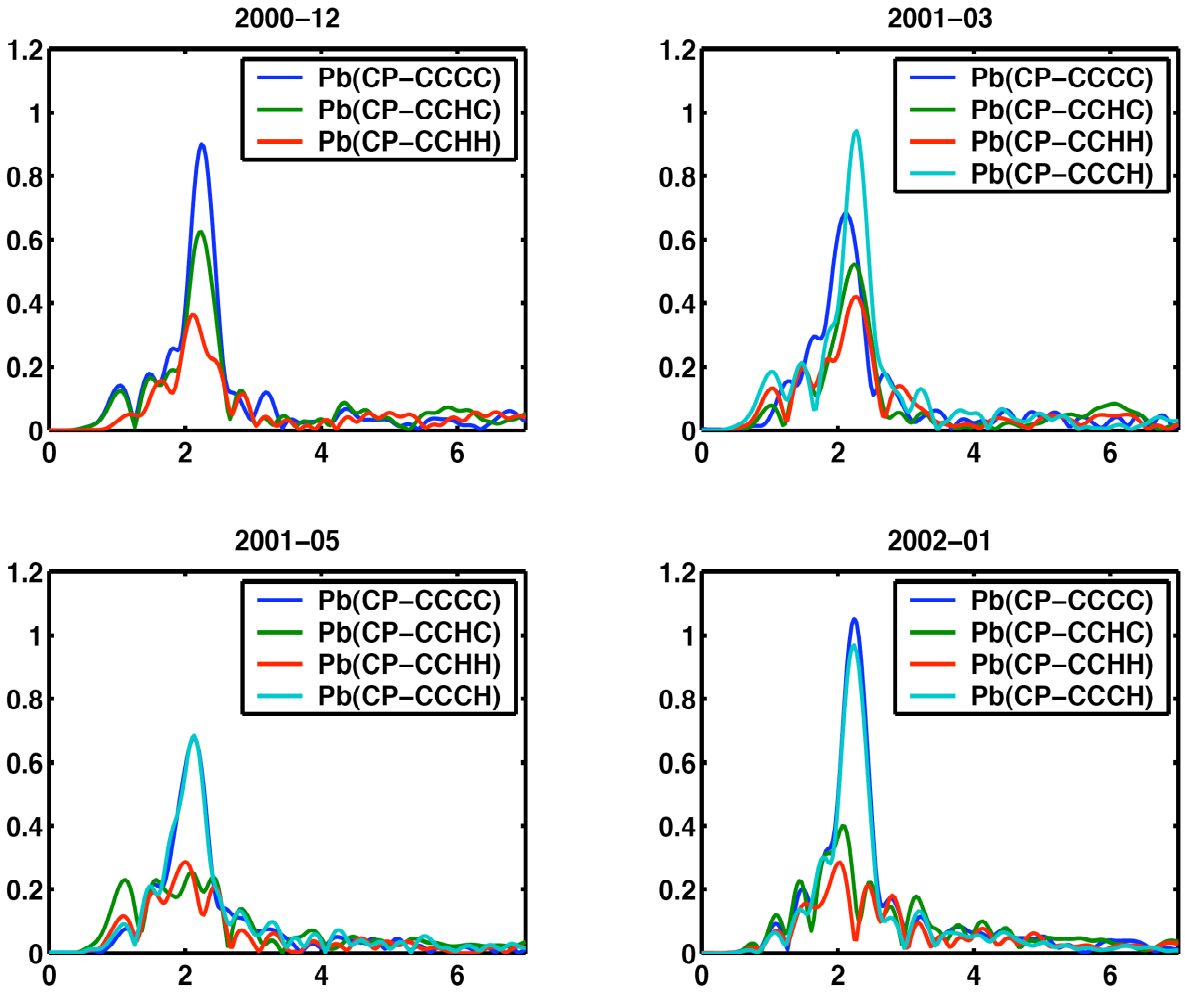

**Figure S3.** Fits using the parameters from Table 2 for the reproducible CP-CCXX data (*i.e.*, the data shown in Fig. 2). Comparable fits were obtained for the HIV-CCHC data.

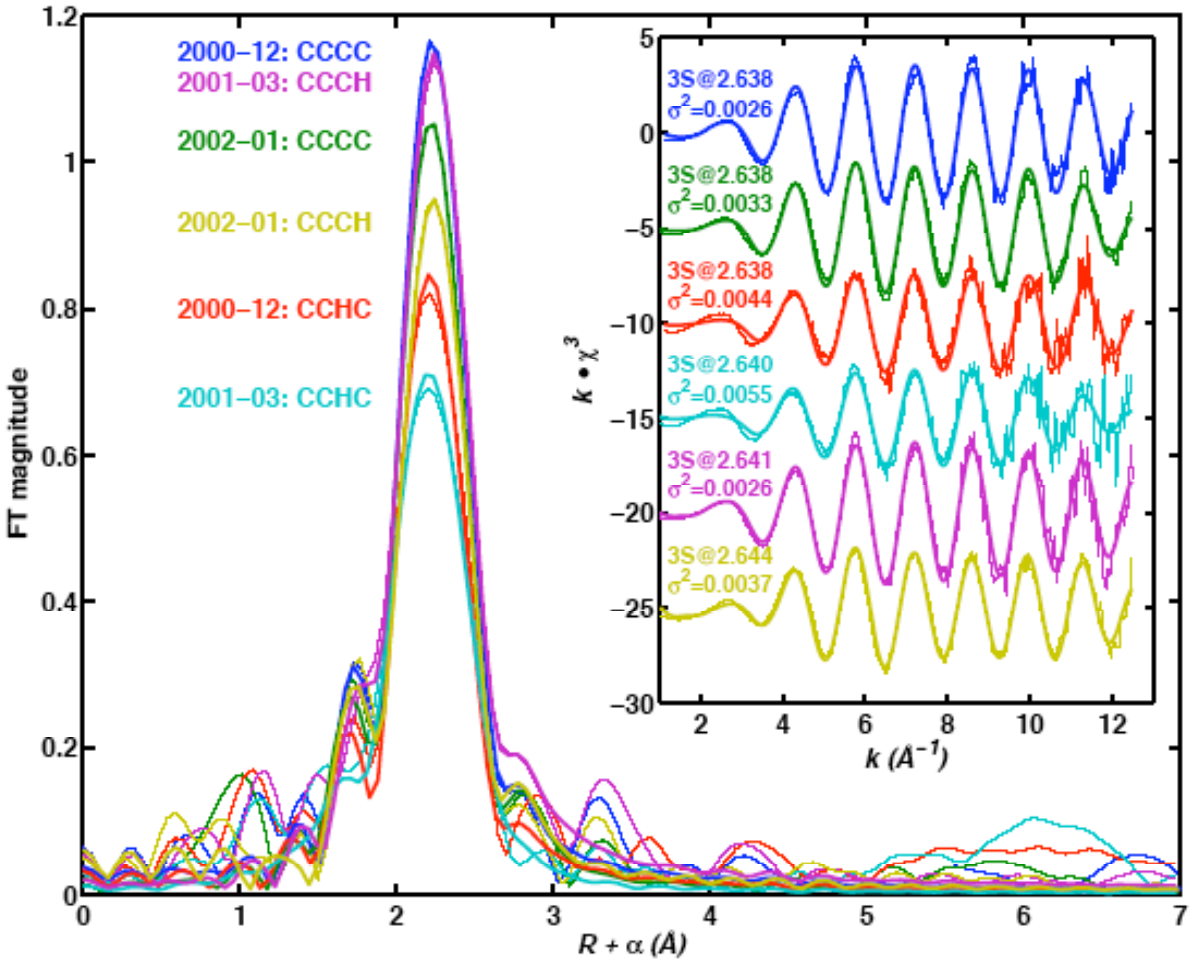

**Figure S4**. UV-visible absorption spectra for the metal-free peptides. These spectral features underlie the data in Figure 4. Top, low temperature (~4 K); bottom, room temperature (~298 K). apo–CP-CCCC (blue), apo–CP-CCCH (green), apo–CP-CCHC (red), apo–HIV-CCHC (black).

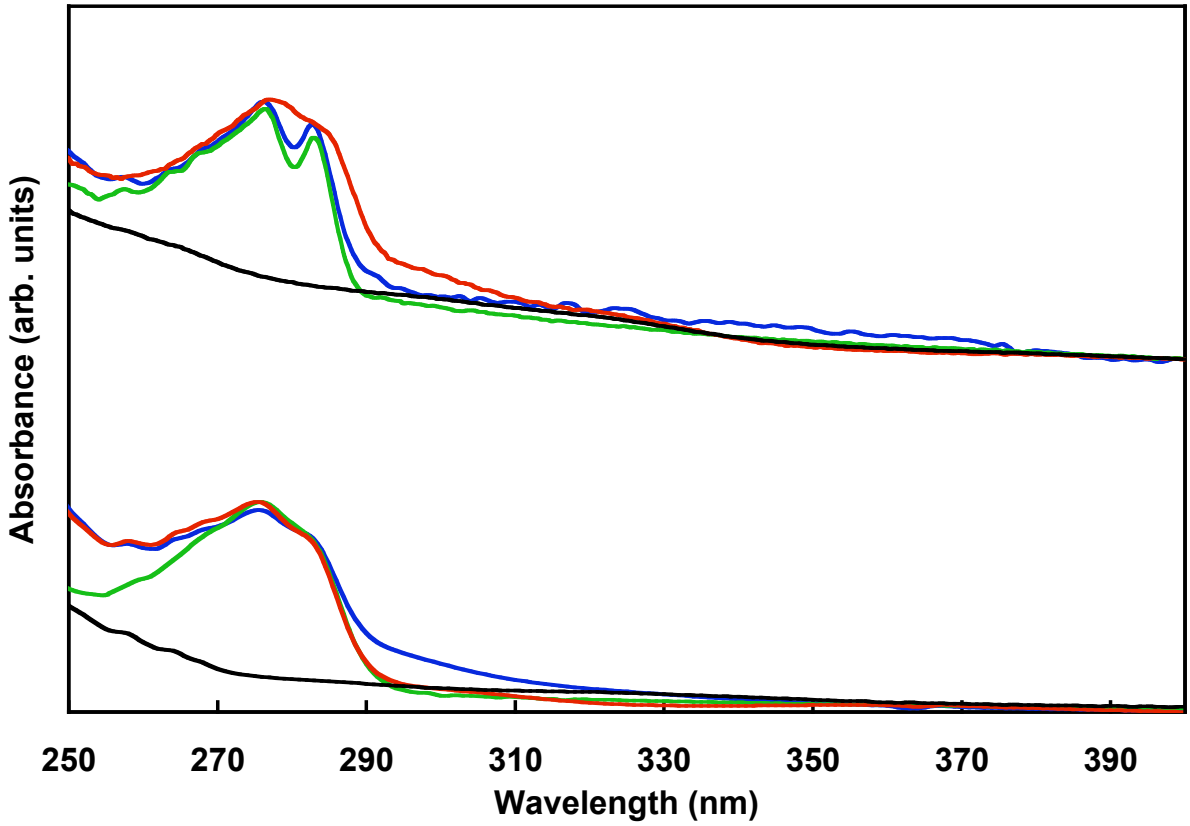

**Figure S5.** Characteristic titration data: UV-vis absorption spectra for titration of Pb–CP-CCCH with Zn(II).

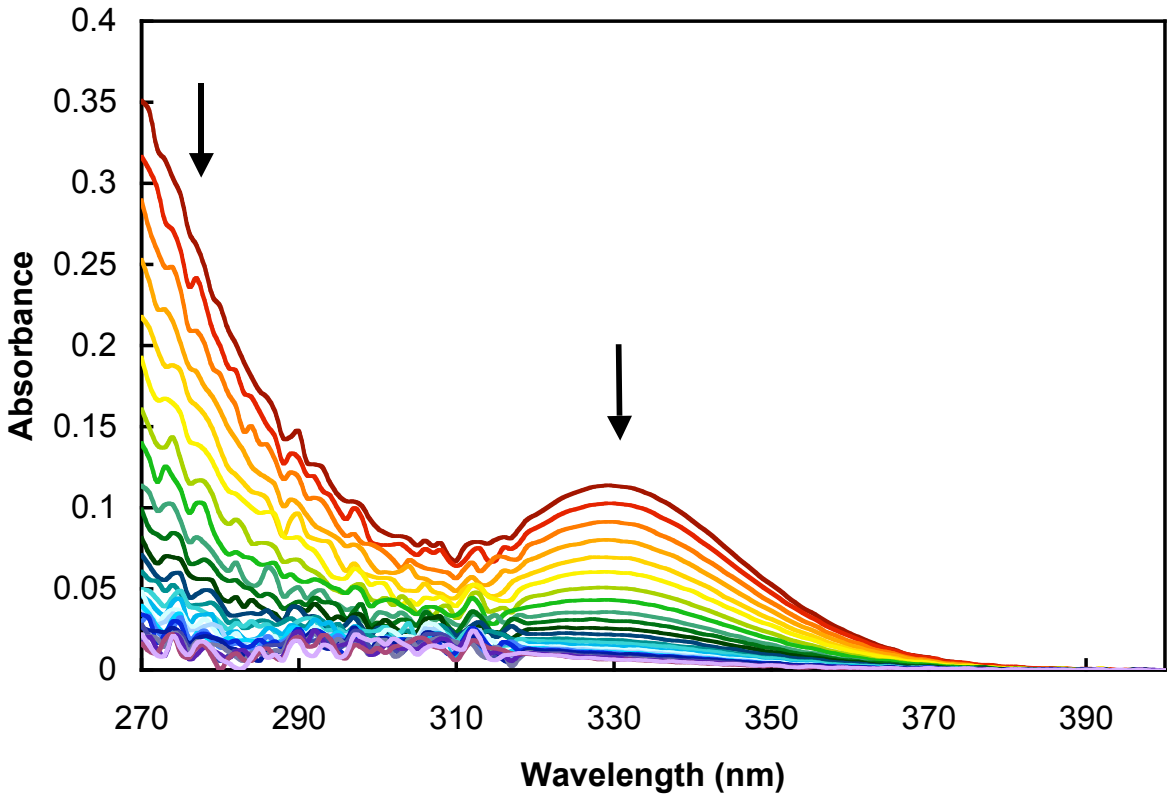

**Figure S6.** Characteristic titration data/fit: absorbance at 330 nm (circles) and fit (solid line) for titration of Pb–CP-CCCH with Zn(II).